

April/May 2014

Science & Technology

REVIEW

WIND ENERGY
IN
THE 21ST CENTURY

Also in this issue:

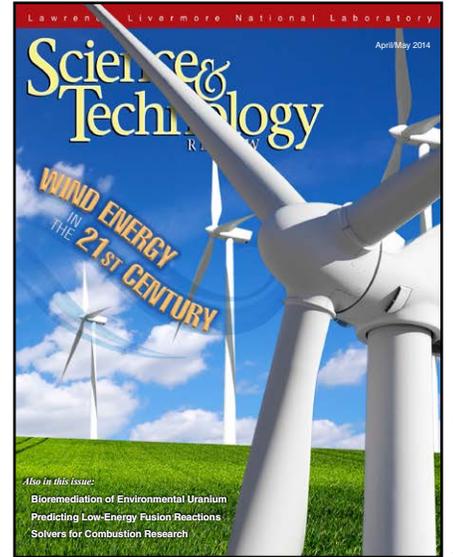
Bioremediation of Environmental Uranium

Predicting Low-Energy Fusion Reactions

Solvers for Combustion Research

About the Cover

Towering farms of wind turbines in America cleanly extract kinetic energy from the wind and convert it to electricity, providing about 4 percent of the total electricity generated in the U.S. President Barack Obama's administration has established a goal of generating 20 percent of the nation's electricity from wind energy by 2030. However, the wind is a variable and uncertain power source that is dependent on many complex atmospheric forces. As the article beginning on p. 4 describes, the goal of the Laboratory's wind-forecasting effort is to reduce the uncertainty in wind power forecasts, on which the wind farm industry and electric power grid operators rely.



About S&TR

At Lawrence Livermore National Laboratory, we focus on science and technology research to ensure our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published eight times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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Contents

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Feature

3 Extracting the Most Energy from Wind
Commentary by Jeff Roberts

4 Predicting Wind Power with Greater Accuracy
A combination of fieldwork, advanced simulation, and statistical analysis is improving wind power predictions to help ensure abundant energy.

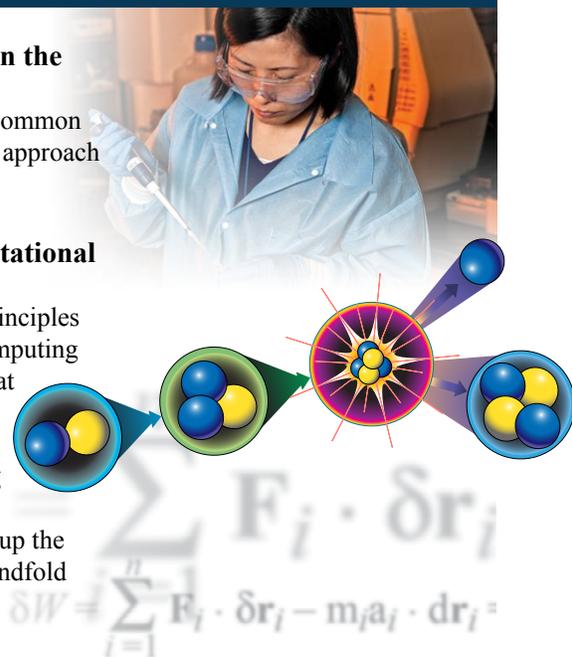


Research Highlights

13 Tiny But Mighty Potential Allies in the Toxic Metal Cleanup Effort
Insights into the survival strategy of a common bacterium may lead to a more effective approach for decontaminating uranium.

17 Nuclear Fusion through a Computational Microscope
Livermore researchers combine first-principles calculations with high-performance computing to model low-energy nuclear reactions at a fundamental level.

20 Chemistry in Motion: Solving Big Problems with an Ultrafast Code
A clever computational method speeds up the modeling of chemical systems a thousandfold over traditional methods.



Departments

- 2** The Laboratory in the News
- 23** Patents and Awards
- 25** Abstract

NIF Experiments Show Initial Gain in Fusion Fuel

Two papers published in the February 5, 2014, edition of *Physical Review Letters* and one published in the February 20, 2014, edition of *Nature* detail a series of National Ignition Facility (NIF) experiments that achieved an order of magnitude improvement in yield performance over past experiments. Ignition—the process of releasing fusion energy equal to or greater than the amount of energy used to confine the fuel—has been a long-term goal of inertial confinement fusion science. A key step along the path to ignition is to have “fuel gains” greater than unity, where the energy generated through fusion reactions exceeds the amount of energy deposited into the fusion fuel. Although ignition remains the ultimate goal, the milestone of achieving fuel gains greater than unity has been reached for the first time ever on any facility.

“What’s really exciting is that we are seeing a steadily increasing contribution to the yield coming from the alpha-particle self-heating, as we push the implosion a little harder each time,” says Livermore physicist Omar Hurricane. In this process, alpha particles—helium nuclei produced in the deuterium–tritium (DT) fusion process—deposit their energy in the DT fuel, rather than escaping. The alpha particles further heat the fuel, increasing the rate of fusion reactions, thus producing more alpha particles. This feedback process is the mechanism that leads to ignition. The process has been demonstrated in a series of experiments in which the fusion yield has been systematically increased by more than a factor of 10 over previous approaches.

The experimental series was designed to limit mixing of the target’s plastic shell with the DT fuel as it is compressed. It was hypothesized that this mixing was the source of degraded fusion yields observed in previous experiments. To suppress the instability that causes mixing, researchers modified the laser pulse used to compress the fuel. The higher yields that were obtained affirmed the hypothesis. The experimental results have matched computer simulations much better than previous experiments, providing an important benchmark for the models used to predict the behavior of matter under conditions similar to those generated during a nuclear explosion, a primary goal for NIF.

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NuSTAR Helps Untangle How Stars Explode

For the first time, an international team of astrophysicists, including Lawrence Livermore scientists, have unraveled how stars blow up in supernova explosions. Using NASA’s Nuclear Spectroscopic Telescope Array (NuSTAR)—a high-energy x-ray observatory—the international collaboration created the first-ever map of radioactive material in a supernova remnant, named Cassiopeia A, or Cas A. (See image below of Cas A captured by NuSTAR.) “One of NuSTAR’s science goals is to map recently synthesized material in young supernova remnants, and Cas A is one of the youngest supernova remnants we know of,” says Mike Pivovarov, a Livermore physicist and coauthor of a paper published in the February 20, 2014, issue of *Nature*.

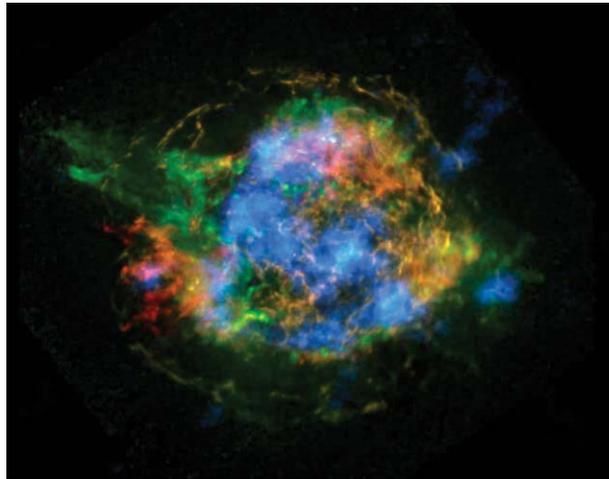
While small stars such as our Sun die less violent deaths, stars with more than eight times the mass of our Sun blow up in core-collapse supernova explosions and create remnants such as Cas A. Because these explosions transform lighter elements into elements heavier than iron, the debris clouds are uniquely responsible for seeding the universe with many heavy elements that are prerequisites for the formation of life on Earth. NuSTAR is the first

telescope capable of producing maps of radioactive material in supernova remnants. In the Cas A study, the material is titanium-44, an atom with an unstable nucleus produced at the heart of the exploding star. “Cas A was a mystery for so long, but now with the map of radioactive material, we’re getting a more complete picture of the core of the explosion,” says Bill Craig, a former Lawrence Livermore scientist now at the University of California at Berkeley and coauthor of the paper.

The NuSTAR map of Cas A, which shows the titanium concentrated in clumps at the remnant’s center, points to a

possible solution to the mystery of how the star met its demise. When researchers have performed computer simulations of supernova blasts, the main shock wave stalls out, and the star fails to shatter. “These latest findings strongly suggest the exploding star literally sloshed around, reenergizing the stalled shock wave and allowing the star to blast off its outer layers,” says Pivovarov, who is part of the optics team along with Livermore’s Julia Vogel and Todd Decker. The optics principles and the fabrication approach for the x-ray optics in NuSTAR are based on those developed for Livermore’s High Energy Focusing Telescope. (See *S&TR*, March 2006, pp. 14–16.)

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Extracting the Most Energy from Wind



THE U.S., along with many foreign nations, is turning increasingly to the power of the wind to meet the rapidly growing demand for clean energy. National security in its fullest meaning must inevitably include energy and environmental security. We must reduce our dependence on imported fossil fuels while ensuring plentiful clean energy with renewable sources. The wind, however, is an intermittent resource that is challenging to predict, sometimes varying significantly from minute to minute. What's more, complex atmospheric factors, such as turbulence, and topographical features, such as hills, modify the wind speed and direction and hence the power that can be extracted by wind turbines. Turbulence also plays an important role in the reliability and life span of turbine components.

As the article beginning on p. 4 describes, Lawrence Livermore scientists and engineers have launched a broad effort to enhance the accuracy of wind power predictions and thereby strengthen America's supply of clean energy. Reducing the uncertainty in wind power forecasts is essential for optimizing power production from wind farms and sustaining the impressive growth of wind energy production in the U.S.

Improving the accuracy of existing wind power models will enable wind farm operators to supply more of the available power to a utility on any given day, improving a utility's capacity factor (the ratio of actual to maximum potential output). Better forecasting and lower uncertainty of wind farm power production also provide an economic benefit to operators, the utilities, and consumers by lowering the cost of energy and enhancing operating profits.

For their part, electric power grid operators need more accurate estimates of power production from wind farms to better match supply with projected customer demand. Every day, utilities depend on a mix of electrical energy sources: traditional baseload (natural gas, nuclear, coal, and geothermal); renewable (primarily wind and solar); storage (hydropower); and standby natural gas plants. With greater certainty of how much power they will receive from wind farms for that day, grid operators will have a better picture for how much they need to tap other energy sources.

To enhance the predictive accuracy of wind power forecasts, Laboratory researchers combine fieldwork, computer simulation, and data analysis. With high-performance computing, a Livermore core competency, we are modeling wind flow and all its perturbations, including turbulence. Our capability in this area has benefited from decades of experience operating the National Atmospheric Release Advisory Center. This facility, which helped

pioneer atmospheric modeling, combines meteorological forecasts and atmospheric dispersion models to predict the probable spread of hazardous material released into the atmosphere and its flow over complex terrain. Wind farms, especially those in the western U.S., are often situated in complex terrains, and models must account for how topography affects the wind.

The simulation challenge can be extraordinarily complicated. For example, simulating the fluctuating power production of an entire wind farm comprising more than 100 turbines requires use of Livermore's massively parallel supercomputers. In addition, the resolved length scales in wind simulations can range from millimeters in the rotor-blade boundary layer to 100 kilometers for large atmospheric weather patterns.

Because we need to validate our simulations, field teams use lidars and other meteorological instruments to collect atmospheric data and measure wind profiles and turbulence blowing into wind farms. We compare those data with the power produced from the turbines during that same time interval to refine power curve models supplied by turbine manufacturers. Refining the power curves can help us more accurately predict power output for a given set of atmospheric conditions.

In our effort to reduce the uncertainty of wind forecasting, we have leveraged expertise originally developed in our nuclear weapons program, which made significant advances in so-called uncertainty quantification, or UQ. By applying UQ, we have identified and narrowed the uncertainties associated with collected field data and with results from various simulation codes.

Wind power is only one component of Livermore's renewable energy portfolio. Our geothermal energy research includes studying where to develop additional reservoirs and how to optimize those reservoirs. We're also investigating new materials for enhanced photovoltaic solar cells and developing better storage technology for hydrogen-powered vehicles. Finally, as more solar and wind resources are added to the grid, we're working with the California Public Utilities Commission to integrate intermittent renewable energy into the electric power grid and help the state prepare for more complex load-balancing situations.

With a full complement of projects, we're working hard to enhance the nation's energy security with a robust mix of renewable and sustainable energy options.

■ Jeff Roberts is the program leader for Renewable Energy and Energy Systems.

Predicting Wind Power with Greater Accuracy

Researchers are combining fieldwork, advanced simulation, and statistical analysis to help wind farm and electric power grid operators.



OVER the past decade, towering farms of wind turbines, some taller than a 40-story building, have become a fixture of the American countryside. These machines, which cleanly extract kinetic energy from the wind and convert it to electricity, today provide about 4 percent of the total electricity generated in the U.S.

President Barack Obama has established a goal of generating 20 percent of the nation's electricity from wind energy by 2030. "We believe it is reasonable to achieve that goal, because of the current high rate of wind turbine deployment nationwide," says Livermore mechanical engineer Wayne Miller, associate program leader for wind and solar power. Between 2008 and 2012, wind power capacity grew by 167 percent. "The market for new wind energy

production is complex and determined by many factors, including federal tax credits for renewable energy production and the availability of cheap natural gas," says Miller. "However, wind is now very competitive with all other sources of power generation that have been recently installed."

Miller notes that the wind is a varying and uncertain power source, dependent on a host of complex atmospheric forces. Reducing the uncertainty in wind power forecasts, on which wind farm operators and electric power grid operators rely, is the goal of a team of Livermore researchers. Many wind farms generate less energy than expected because of uncertainties in forecasting winds and in simulating the complex flows within the turbine farms. Greater understanding

of the wind is needed to optimize power production from these farms and to improve the fidelity of forecasting models that relate power output to atmospheric conditions. A major focus for the team is to better understand how power production is related to atmospheric variables, such as wind speed and turbulence, across a broad range of spatial and temporal scales and in widely varying geographic areas.

The Laboratory's wind-forecasting effort involves about a dozen atmospheric scientists, mechanical and computational engineers, and statisticians who combine fieldwork, advanced simulation, and statistical analysis. "It's a big team effort," says Miller. Partners include the National Renewable Energy Laboratory, National Center for Atmospheric Research,



University of Colorado at Boulder, Sandia and Pacific Northwest national laboratories, University of Wyoming, University of Oklahoma, University of California at Berkeley, U.S. Army, and the wind power industry. Funding is provided by the Department of Energy’s (DOE’s) Office of Energy Efficiency and Renewable Energy, Livermore’s Laboratory Directed Research and Development (LDRD) Program, and industrial partnerships.

The team’s advanced numerical models, verified by fieldwork and statistical analysis, account for atmospheric complexities both horizontally across landmasses and vertically above Earth’s surface. High-resolution computer simulations provide useful data to wind farm developers and operators, enabling them to better select wind farm locations and operate the sites with increased efficiency. Improving the accuracy of wind predictions is also critical to electric grid operators who must dynamically balance the variable power generated by increasing or decreasing power production from other sources such as coal, natural gas, hydroelectric, geothermal, and biomass.

Observations Feed, Verify Simulations

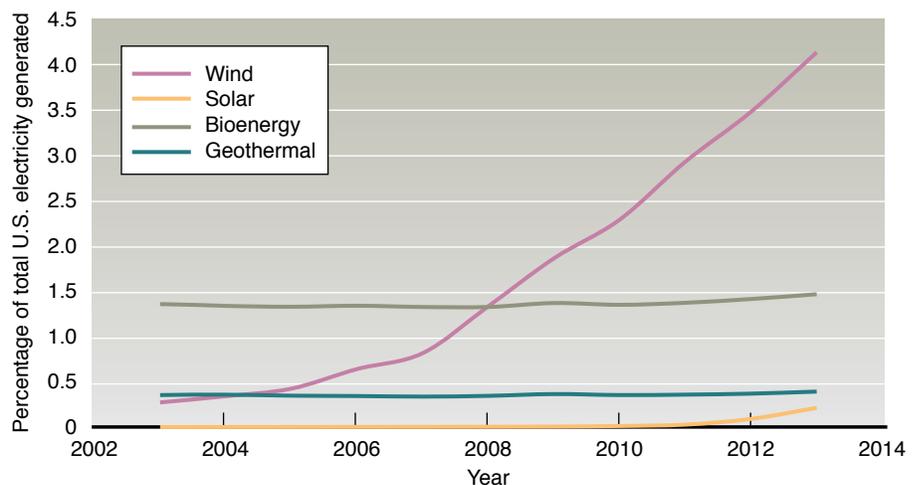
Livermore field researchers are characterizing winds in numerous locations across the U.S. and are especially focused on understanding the flow in the Altamont Hills just east of Livermore, California—an area populated with wind farms. They have made significant findings studying the dynamics of atmospheric instability and turbulence. Turbulence is a particularly important variable because it affects the amount of power extracted from wind turbines as well as the reliability and life span of turbine components.

The Livermore researchers compile wind data from stationary towers mounted with weather instruments. They also use high-resolution, remote-sensing instruments including sodar and lidar to provide vertical profiles of wind speed, direction, and turbulence in the lower layer of the atmosphere. These data are collected at numerous sites such as Lawrence Livermore’s Site 300 experimental research facility located about 20 kilometers east of the Laboratory’s main site, DOE’s Southern Great Plains Atmospheric Radiation Measurement Climate Research Facility in Oklahoma, and wind farms in the Altamont Hills and northern Oklahoma.



Jennifer Newman, a University of Oklahoma graduate student funded by Livermore’s Laboratory Directed Research and Development Program, checks on a solar-powered lidar station at a wind farm near Lawrence Livermore. Lidar stations provide vertical profiles of wind speed, direction, and turbulence in the lower layer of the atmosphere.

Today, wind power provides about 19 gigawatts, or about 4 percent, of the total electricity generated in the U.S. The Obama administration has established the goal of generating 20 percent of the nation’s electricity from wind energy by 2030.



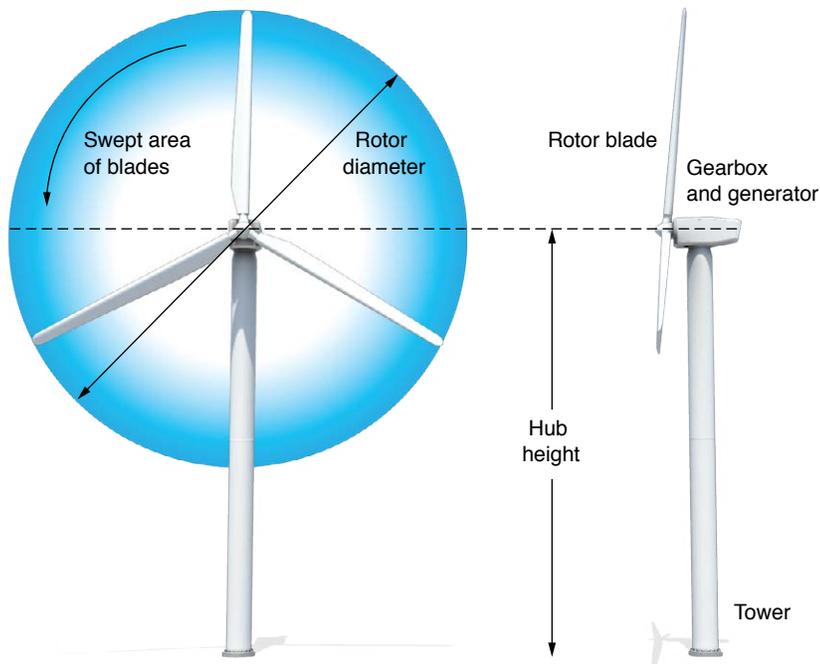


Atmospheric scientist Sonia Wharton explains that wind turbines operate in the first 150 meters of the 1-kilometer-high atmospheric boundary layer. In this layer adjacent to the ground surface, a significant exchange of heat occurs between the surface and atmosphere during daytime, which induces turbulence. Friction from the wind moving over hills, trees, and buildings also induces turbulence.

Wharton notes that as deployment of wind farms has increased, so have the average turbine hub height (distance from the ground to the blade rotor), blade diameter, and power-generating capacity. Taller turbines typically encounter higher wind speeds, allowing them to extract greater amounts of energy. Tall turbines also experience more complex airflow patterns driven by turbulent mixing. Although the average wind speed in the blade-swept area largely determines the amount of power generated (power is proportional to the cube of the wind speed), wind shear and turbulence also affect power output. For example, wind speeds can vary significantly at opposite ends of the blades, which can cause the blades to twist and deform, reducing power output and causing premature wear.

“Our measurements help us better understand the physics of the atmospheric boundary layer,” says Wharton. “Increased understanding can help optimize power generation from wind farms and validate our numerical models.” Wharton uses wind profile data to investigate stability factors, including vertical and horizontal turbulence intensity, veer (change in direction with height), and shear (change in wind speed with height). She compares those data to supervisory control and data acquisition (SCADA) information remotely transmitted from turbines. SCADA data, typically generated at 10-minute intervals, provide many turbine performance factors, including the yaw angle as the nacelle points to the wind, the blade pitch angle (which controls rotor speed and torque), hub-height wind speed, and power. Her research, in collaboration with scientists at the University of Oklahoma and the University of Wyoming, involves some of the most detailed studies to date exploring the relationship between three-dimensional turbulence and turbine power production.

Field studies at Site 300 and at an Altamont Hills wind farm focus on



As wind turbine blades rotate, they spin a shaft, which is connected to an electric generator. Wind turbines include a gearbox to increase the spinning shaft's speed from about 30 to 60 revolutions per minute (rpm) to the 1,000 to 1,800 rpm required by most generators to produce electricity. The hub height of most land-based turbines ranges from 60 to 100 meters. Rotor diameters can exceed 120 meters. (Rendering by Kwei-Yu Chu.)

understanding the complex wind patterns occurring in a hilly, coast-influenced region—a location similar to that of many California wind farms. Scientists have also analyzed wind profiles at flat-terrain sites in the nation, such as the very windy Great Plains, to study low-level jets and other drivers of complex atmospheric flow. “These jets, which are similar to a river of very fast air, occur at night in the Plains states and provide more power than higher level jets,” says Wharton. With improved characterization of the interactions between particular inflows and turbines over a variety of terrains, scientists and engineers can better model and design turbines for optimal performance.

Along with Laboratory atmospheric scientist Matthew Simpson and industry collaborators, Wharton is also using lidar data to study how power generation is affected by a wind ramp, which is a significant change in wind speed over just a few hours. “Our work underscores the benefit of observing complete profiles of wind speed and turbulence across the turbine rotor disk, which is available only with remote-sensing technologies such as sodar and lidar,” says Wharton. She notes that wind turbine manufacturers typically provide operators with a “power curve,” a graph that shows power from the turbine as primarily the cube of hub-height wind speed alone.

“Power curves oversimplify reality,” says Wharton. “In fact, they frequently err by plus or minus 20 percent of actual power output. We’re adding refinements to power curve models so that they reflect our knowledge of the aerodynamic environment. The more we understand atmospheric processes, the more accurate our power predictions.”

Simulations Face Challenges

Livermore’s wind-forecasting simulation and modeling efforts rely on massively parallel supercomputers to study atmospheric flows relevant to wind farm

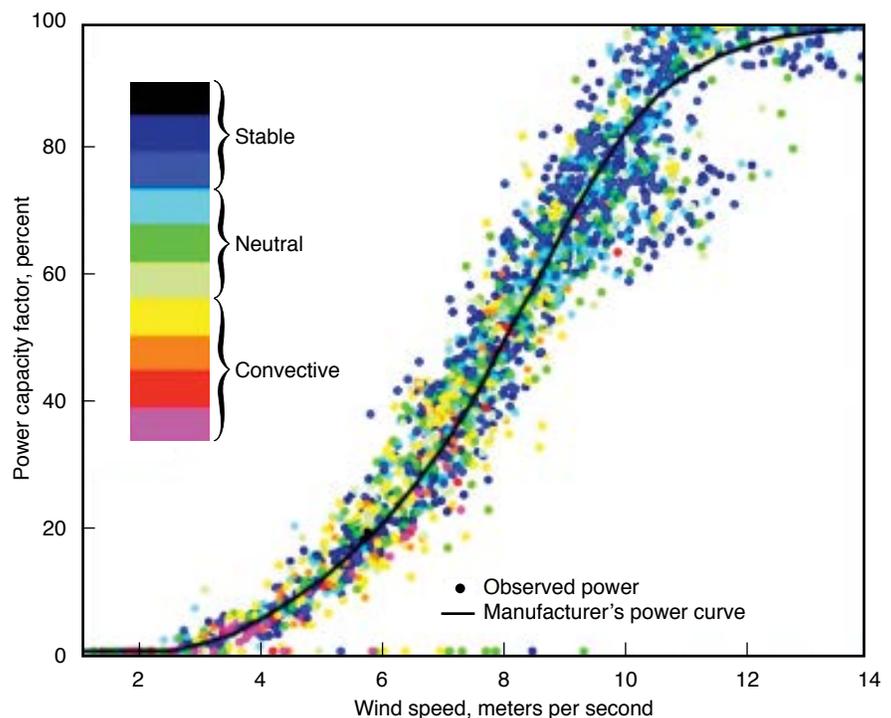
operations. The task is enormous because the length scales involved can span eight orders of magnitude—from the mesoscale (about 100 kilometers) to wind farm scales (1 to several kilometers) to turbine blade aerodynamic features (millimeters to meters).

“Simulating wind change and its effects on turbines is challenging because of the complex forces driving wind,” says Miller. “We’re essentially simulating a fluid flow in an environment where factors such as aerosols, clouds, humidity, surface-atmosphere energy exchange, and terrain influence to varying degrees both the complexity of the flow and how much power can be extracted by a spinning turbine.” Turbine rotors spin via aerodynamic forces (lift and drag) imparted to the blades when air flows

over them. The blades are attached to a shaft that, in turn, spins a generator to produce typically between 1.5 and 3 megawatts of power at full speed in land-based turbines.

Modeling the atmospheric forces that drive the wind as it acts on a single turbine poses a significant computational challenge. The job is vastly compounded when attempting to model a wind farm with 100 or more turbines. What’s more, simulations must account for varying terrain that can significantly affect power output from one wind turbine to the next. They must also account for turbulent wakes from the front rank of spinning turbine blades, which can rob power from turbines downstream.

“Because of the complexity of wind patterns and the huge range of



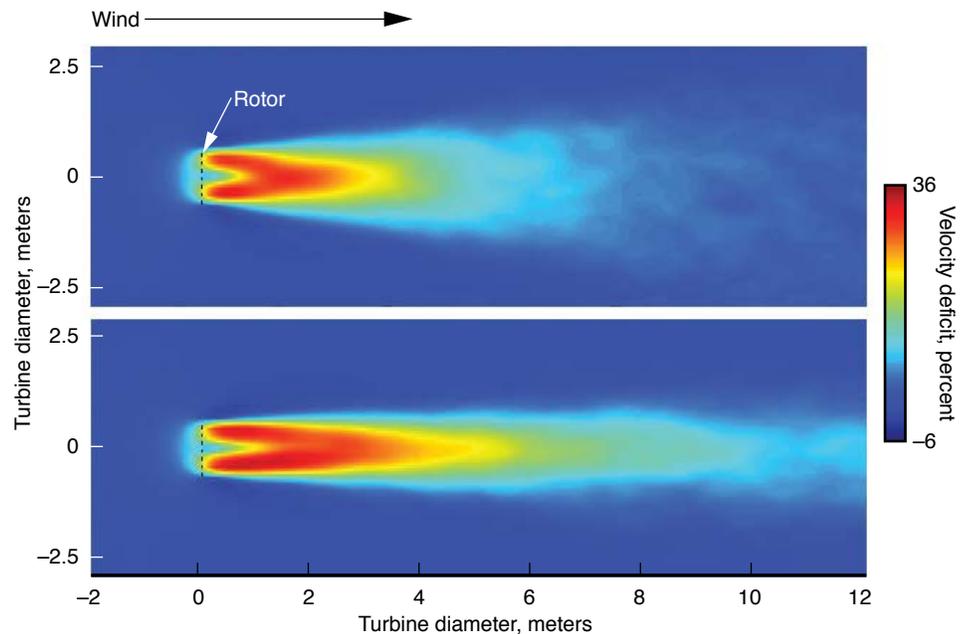
Wind turbine manufacturers typically provide operators with a simple “power curve,” which shows power from the turbine as primarily the cube of hub-height wind speed. However, Livermore researchers are showing that power curves frequently err by ± 20 percent of actual power output, as seen in this plot of observed power versus wind speed at a northern California wind farm. The color map relates atmospheric stability conditions to reported power-output observations.

relevant scales, the computational task of simulating a wind farm is daunting,” Miller says. To address knowledge gaps and research challenges associated with these simulations, atmospheric scientist Jeff Mirocha and others are extending the applicability of the Weather Research Forecasting (WRF) modeling system to the wind farm scale. This popular model, maintained collectively by more than 10,000 users and contributors worldwide, was developed primarily for larger-scale weather applications.

Mirocha says, “We have modified WRF extensively to make it applicable to the smaller scales. Accurate wind power forecasts often require a multiscale simulation approach to account for all the important scales.” As an example of multiscale methodology, one can begin with a simulation of the western U.S. to capture the evolution of large-scale weather patterns. Thereafter, a combination of smaller grid spacing and Livermore-developed submodels can accurately resolve the additional smaller-scale features that affect wind farms.

Once smaller scales of flow are resolved, wind turbine models can be implemented to investigate processes important to engineering applications such as wakes, power production, and turbine component fatigue. “Wind power simulation lies at the boundary of engineering and atmospheric sciences,” says Mirocha, who is attempting to seamlessly blend WRF atmospheric simulation with scales of motion traditionally handled by computational fluid dynamics (CFD) codes. Typical CFD codes do not contain representations of many important atmospheric physical processes contained within WRF. The complex interactions of these physical processes can strongly modulate the flow entering a wind farm and therefore the power produced or fatigue experienced by turbines.

To capture the interactions between wind turbines and complex atmospheric



Two simulations of a Generalized Actuator Disk wind turbine model within the Weather Research and Forecasting (WRF) code depict the wake downstream from a wind turbine rotor plane (dashed line). The simulations, viewed from above looking down at the turbines, show how the strength of background atmospheric turbulence (convective instability) influences turbine wakes. Stronger turbulence (top) attenuates the wake more rapidly than weaker turbulence (bottom).

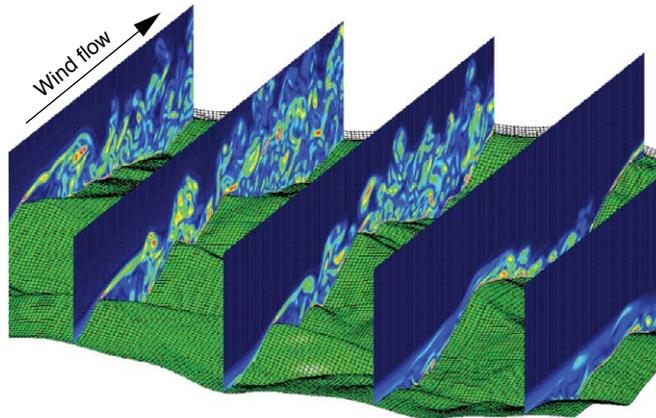
flows, Mirocha implemented a Generalized Actuator Disk (GAD) wind turbine model within WRF. GAD, an approach typically used in engineering CFD codes, depicts a two-dimensional disk containing a rotating turbine. Lift and drag forces on the turbine blades respond to atmospheric flow, including the effects of large eddies (swirling vortices of air). GAD calculates the power output of a front-rank turbine rotor and the effects from wakes that emanate downstream. These wakes, which feature both reduced wind speeds and increased turbulence, are of key concern because they are associated with power losses of up to 40 percent, and they shorten the operational life span of turbine components. WRF-GAD is being extended to a model that resolves each turbine blade independently, which will provide higher fidelity representations of blade-airflow interactions. In addition, a structural response model is being implemented within WRF to investigate

turbine fatigue in response to wakes and atmospheric turbulence.

The downscaling capability in combination with these engineering submodels will allow researchers to study a variety of phenomena unique to the wind farm environment. Says Mirocha, “The simulation framework we are developing will provide advanced tools to address these knowledge gaps, leading to improved operations, longer component life spans, and ultimately cheaper electricity.”

In addition to atmospheric physics, complex terrain can also influence the flow and turbulence experienced by wind turbines. “Eddies in the atmosphere spin and twist similar to water passing over rocks in a fast-moving stream,” explains computational scientist Kyle Chand. “A wind farm design must account for how wind is influenced as it flows past a particular terrain.” Because the standard WRF model was designed primarily for larger scales, it was restricted to simple

A simulation using Livermore's CGWind code shows the evolution of large eddies as they propagate over complex terrain at the Laboratory's Site 300 experimental research facility. The wind flows in the direction of the simulated slices, from lower left to upper right. The colors denote the strength of the turbulence, with red representing the strongest.



terrain with shallow slopes. However, an additional Livermore-developed approach, the immersed boundary method (IBM), eliminates this restriction.

The researchers combined WRF and IBM to simulate wind over hills and other complex terrains such as Oklahoma City. Says mechanical engineer Katie Lundquist, who developed IBM for her dissertation, "IBM allows us to use a Cartesian grid. Working with grids as small as 1 meter, we can accommodate, for the first time, simulations of flow in mountainous terrain with nearly vertical slopes without compromising accuracy." With DOE and LDRD funding, Lundquist is now refining the code.

Two additional codes, CGWind and HELIOS, are used for even smaller-scale simulations that would be impractical

with WRF. With CGWind, which Chand developed in 2009 with LDRD funding, topological features such as hills, buildings, and wind turbines can be accurately modeled. In addition, finer grids can be overlaid for areas requiring higher resolution, allowing the code to focus computational resources only where they are needed. CGWind has been used to model wind over a number of complex terrains, including the Laboratory's hilly Site 300.

HELIOS is a multiphysics rotor aerodynamics CFD code originally developed by the U.S. Army to model helicopters. The code was later adapted for wind turbines by the University of Wyoming. "Essentially, our colleagues at Wyoming turned the Army code for helicopters sideways to capture the tiny

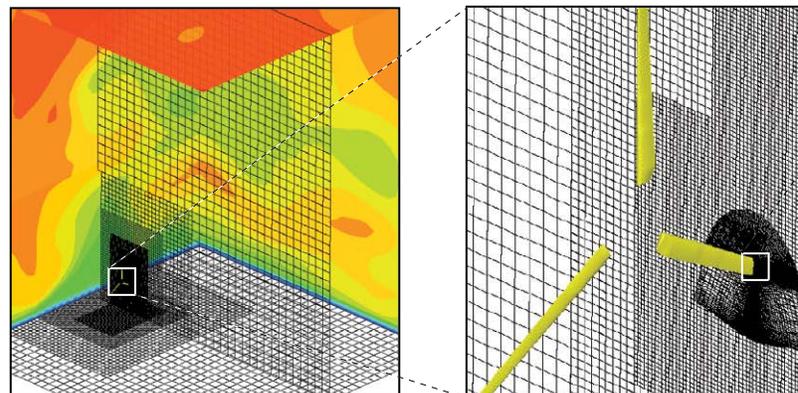
vortices created at the tips of turbine blades and to model structural loads," says Miller. In collaboration, Livermore and Wyoming have used HELIOS to perform the first-ever simulation of a 50-turbine wind farm that resolves individual spinning turbine blades. The team is extending this effort using a Livermore Computing Grand Challenge Award to run simulations of a 150-turbine farm. The simulations combine WRF and HELIOS and require up to 100,000 cores (processors working together) on the Laboratory's Vulcan supercomputer.

Minimizing Uncertainties

Another group of Livermore researchers is studying how to reduce uncertainties in the errors associated with collected field data and with the assumptions, inputs, and approximations inherent in the physics of the WRF code, its constituent modules, and the nested CFD codes. Their work takes advantage of the Laboratory's strength in statistical modeling and uncertainty quantification (UQ), which has proved invaluable in stockpile stewardship.

"Wind power forecasting involves converting atmospheric forecasts into a forecast of power output from an individual turbine or many turbines in a wind farm," says statistician Vera Bulaevskaya. Traditional manufacturer-supplied power curves model power as a function of the wind speed at the hub

Livermore and University of Wyoming simulation experts combined the WRF model with HELIOS to perform the first-ever simulation of a 50-turbine wind farm that resolves individual spinning turbine blades using realistic turbulent winds. Such realism is needed to understand how wind farms often underperform in real situations compared with idealized results. Colors show WRF wind velocity variations flowing into the HELIOS turbine grid.



height of the turbine (adjusted for air density). In reality, however, power output is a function of additional variables. For example, wind speed at heights below and above the hub, wind shear, and turbulence are also strong predictors of power production. Accounting for them provides a more complete power curve model. Bulaevskaya compares lidar atmospheric data collected at wind farms with SCADA power output data from wind turbines to gain a detailed understanding of the sensitivity of power output to changes in atmospheric conditions.

Moreover, to be valuable, a forecasting tool must not only produce accurate forecasts of power but also correctly quantify the uncertainty, or confidence level, associated with these predictions. Such confidence levels are particularly of value to electric grid operators, who need both the predictions of output and the associated levels of confidence to determine an optimal schedule for turning various sources of power on and off. Quantifying output uncertainty is also crucial for siting wind farms.

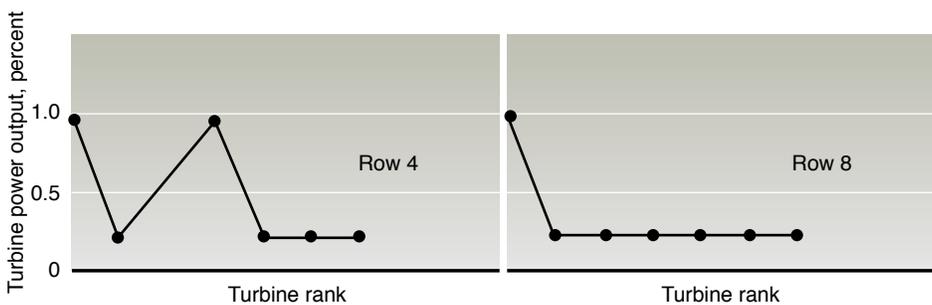
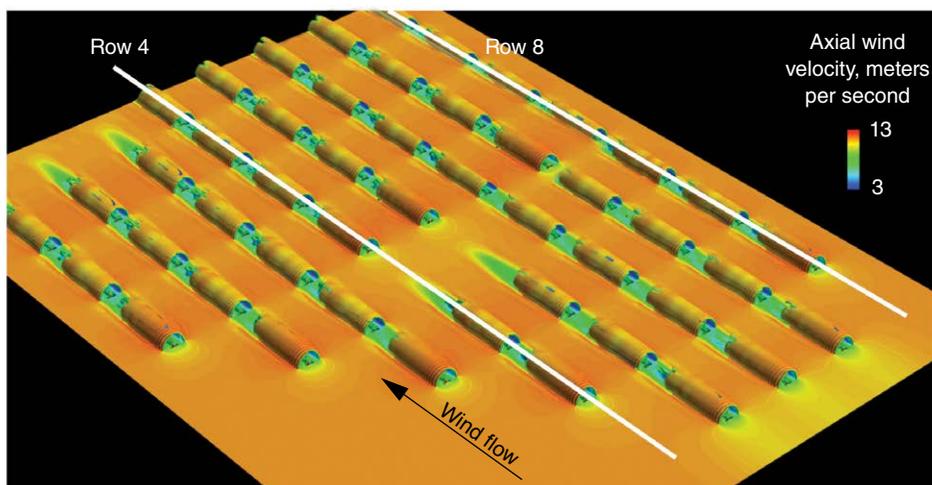
Bulaevskaya has investigated various statistical approaches for modeling power as a function of changes in atmospheric conditions. She has found that the performance of these approaches, in terms of prediction accuracy, is significantly better than that of manufacturers' power curves. (See the figure on p. 12.) One

statistical technique, known as the Gaussian Process Model, is particularly well suited for estimating the uncertainty associated with predictions.

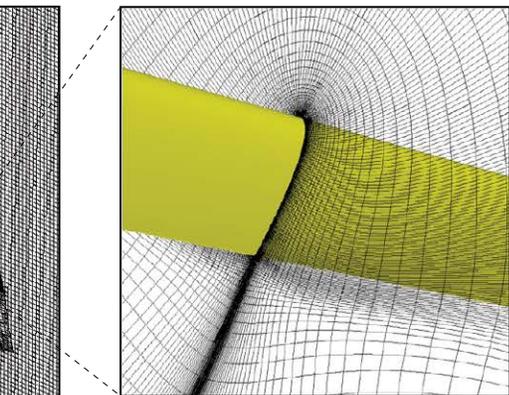
Ultimately, forecasts of atmospheric variables, rather than observed values, will be used to predict output. To reduce uncertainties in these forecasts, Simpson performs "ensemble modeling," which entails running a wind forecast model dozens or even hundreds of times using slightly different starting conditions and physics packages or submodels. (See *S&TR*, December 2013, pp. 20–23.) One ensemble can constitute 30 to 60 runs of slightly different WRF models—a process

that requires significant supercomputing resources. He explains that WRF contains many individual packages, each representing a particular atmospheric physics component, such as a model of turbulence or clouds. These packages provide descriptions of physical processes developed by different researchers. To account for a full range of physical phenomena, Simpson varies the packages within WRF.

To model wind power predictions, Simpson begins with forecasts of atmospheric variables. The initial input is uncertain. Factors such as temperature, wind, air pressure, and large-scale weather



(top) The effect of downstream wakes caused by upstream wind turbines is illustrated in this HELIOS simulation of an offshore wind farm in Denmark. (bottom right) In row 8, turbine power is at 100 percent in the first turbine but quickly falls off because of the downstream wake. (bottom left) In row 4, the wind "recharges" in the gap after the second turbine, allowing the third turbine to produce nearly maximum power.



features ultimately affect much smaller areas such as wind farms. By running numerous simulations with a plausible sampling of varying physics packages and initial conditions, researchers obtain a range of outcomes. A set of predictions resulting from these model ensembles can then be used to quantify the uncertainty in the predictions resulting from incomplete knowledge about atmospheric physics and model inputs.

One advantage of ensembles is the capability to spot outliers such as wind ramps. Because power output is proportional to the cube of the wind speed,

a wind ramp can result in a dramatic change in power production. Consequently, accurate wind ramp prediction is extremely important, leading some experts to refer to it as “the Holy Grail of wind forecasting.” In one case study, an ensemble run showed that the ability to predict a wind ramp did not improve with grid resolution finer than 1 kilometer. Results such as these can help guide researchers to use computer resources more efficiently and further refine models.

Atmospheric scientist Don Lucas has worked extensively with climate and atmospheric model uncertainties and has

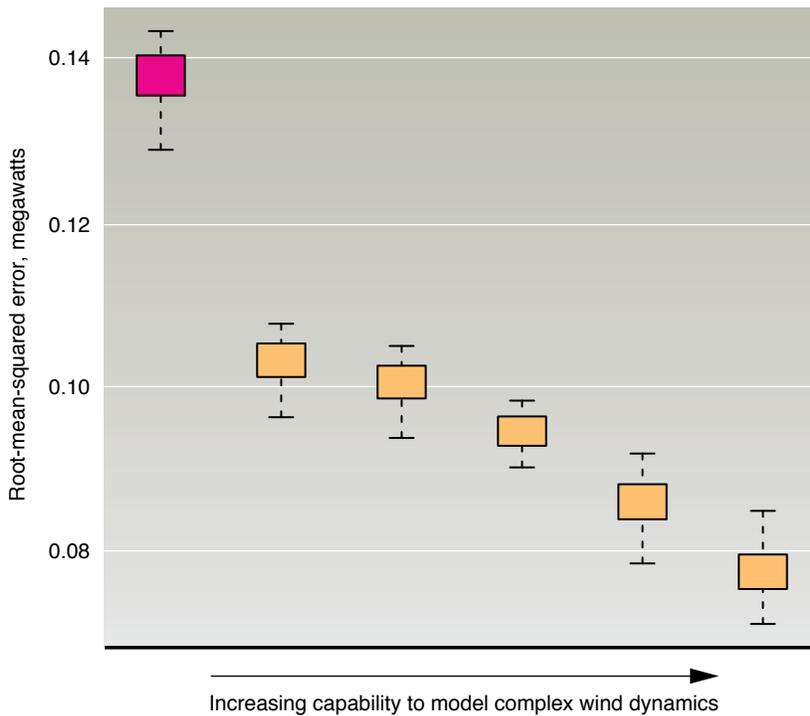
run thousands of ensemble simulations during his career. “UQ is at the interface of computer simulation and statistical analysis,” he says. “Sometimes, changing parameters or their relative strengths does not affect the output or exerts only a small influence. We can determine which factors greatly influence forecast and focus computational resources on those.” At the same time, he notes that relevant field data help keep models “honest.” “We want to improve UQ calculations with observations to see how well we know the model and how well the model performs.”

Benefits of Accurate Predictions

Together, the field observations, simulations, and statistical analyses are significantly improving wind power predictions. The Laboratory is sharing the results of this work with the wind industry to help turbine manufacturers refine their power curves and incorporate findings about what atmospheric processes are important in wind power forecasting.

With improved models, wind farm operators will know how to better maximize their sizable investments, more skillfully bid into the energy market, optimally site turbines, and minimize the turbulent wakes from upstream turbines. The biggest winner, however, may well be the American consumer, who will enjoy abundant supplies of energy from a clean and inexhaustible source.

—Arnie Heller



As statistical models account for increasingly complex information about wind dynamics, the root-mean-squared error associated with predicted power output from a wind turbine decreases significantly. Livermore researchers used lidar data as input to five power curve models (gold squares) and compared their results with a manufacturer’s power curve (pink square) for a number of data sets. The power curve models incorporating successively more information about wind dynamics tended to have a much lower prediction error.

Key Words: atmospheric boundary layer, CGWind, computational fluid dynamics (CFD), electric power grid, Gaussian Process Model, Generalized Actuator Disk (GAD), HELIOS, immersed boundary method (IBM), lidar, mesoscale, sodar, supervisory control and data acquisition (SCADA), turbulence, Weather Research Forecasting (WRF), wind turbine farm, wind power forecast.

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Tiny But Mighty Potential Allies in the Toxic Metal Cleanup Effort

THE Department of Energy (DOE) is tasked with cleaning up roughly 120 sites in the U.S. and its territories that are contaminated with depleted uranium and other toxic heavy metals as a result of energy and weapons production activities. Without treatment, these metals will persist and accumulate in the food chain. High cost and concerns about long-term effectiveness hamper the widespread application of current chemical and physical remediation methods. Bioremediation—using naturally occurring or genetically modified organisms to detoxify hazardous substances—potentially offers an efficient, inexpensive, and environmentally friendly alternative. While even trace amounts of uranium pose a threat to human and animal health, some bacteria tolerate environments with surprisingly high uranium concentrations. Scientists are working to understand the natural coping mechanisms of these microorganisms so they can be exploited at contaminated sites.

Livermore microbiologist Yongqin Jiao is midway through a five-year study, funded by DOE's Early Career Research Program, to investigate how certain aerobic bacteria interact with uranium in aquatic environments. She is focusing on the metabolic processes of the common bacterium *Caulobacter crescentus*, which tolerates low-nutrient environments, including uranium-contaminated groundwater. Because

Livermore postdoctoral researchers Dan Park (left) and Mimi Yung (right) study bacteria samples that are missing a critical gene for survival in the presence of uranium. (Photograph by George A. Kitrinis.)

other research groups have extensively studied the genome and life cycle of *C. crescentus*, the bacterium serves as an ideal model system. In a series of experiments, Jiao and her colleagues found that *C. crescentus* reduces the toxicity and mobility of the uranium in the bacterium's environment. Jiao's work to illuminate the survival strategy of *C. crescentus* supports DOE efforts to better understand the natural processes occurring at contaminated sites and ultimately to improve uranium remediation approaches.

Arresting Behavior

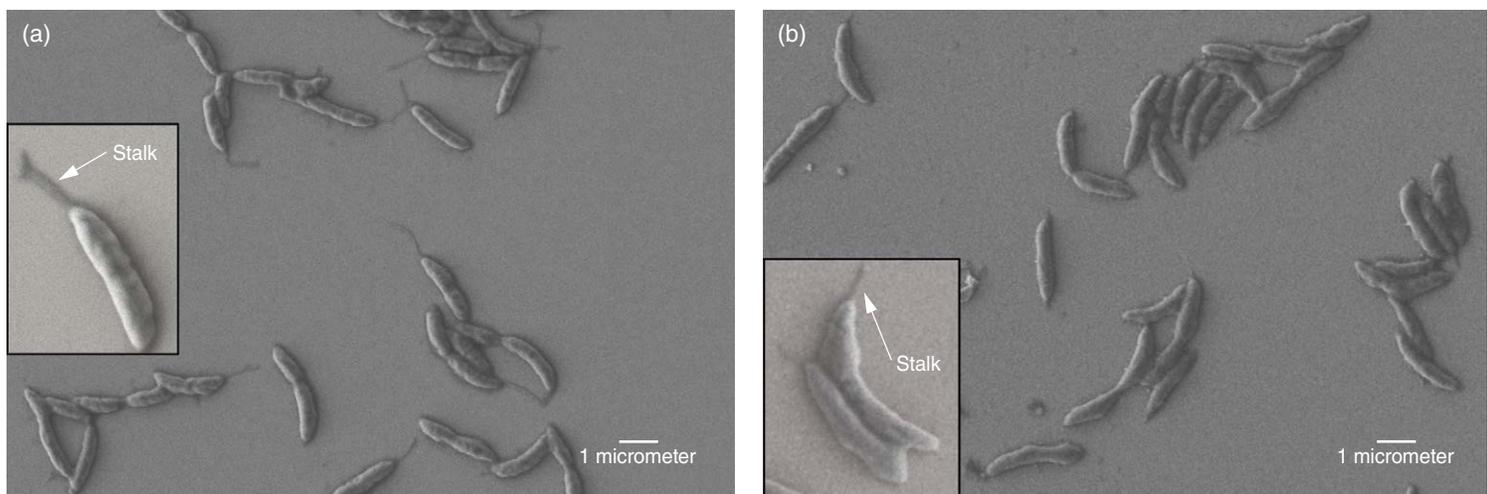
When *C. crescentus* is added to a test tube containing growth media, the bacterium normally begins multiplying immediately. However, when the Livermore team added *C. crescentus* to a growth medium that also included uranium, the bacterium experienced an initial period without population growth. The duration of the no-growth period was proportional to the concentration of uranium. Once *C. crescentus* began growing, it grew at the same rate and to the same final population density as cells not exposed to uranium. The researchers examined the cells during the no-growth phase using scanning electron microscopy (SEM) and found that the cells' development appeared to stall.

Understanding what occurred during this period seemed essential to explaining the bacterium's uranium tolerance. To investigate whether the reaction of *C. crescentus* to uranium was unique, the researchers exposed the bacterium to eight other heavy metals. Zinc was the only other metal that produced the characteristic pattern of growth arrest, followed by normal growth and yield. The team also introduced uranium into cultures of three common soil- and gut-dwelling microbes—including one

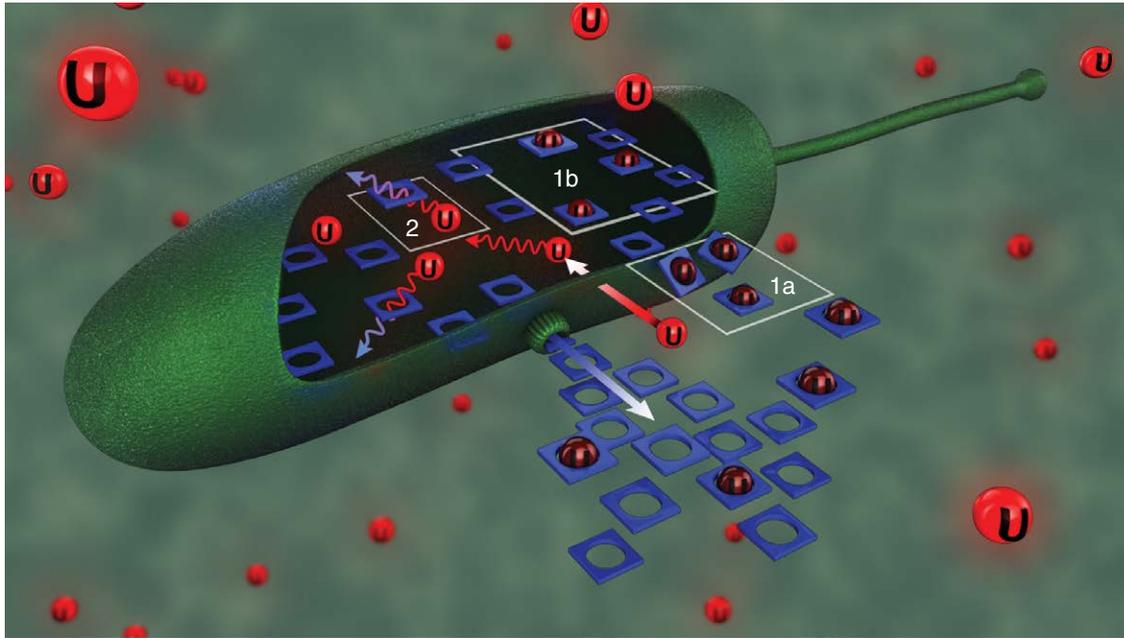
known for its heavy metal resistance—to compare their responses. The researchers were surprised to find that *C. crescentus* had by far the shortest growth arrest period. Notes Jiao, "The other species experience a lengthier growth arrest because they are not as resistant to uranium toxicity. However, those species are likely interacting with the uranium through similar mechanisms, so what we learn about *C. crescentus* may be applicable to other aerobic bacteria."

The team then explored whether the bacterium was somehow altering its environment during this phase. Researchers removed the growth media from *C. crescentus* cultures at different points in the growth-arrest phase and placed the media in new cultures of *C. crescentus*. They found that growth arrest is reduced when the growth media is reused. Arrest periods are shortest in cultures with media collected from late in the no-growth period. In collaboration with biologist Lucy Shapiro at Stanford University, the researchers also monitored expression of a *C. crescentus* gene region previously shown to specifically sense uranium. The team noted that the uranium sensor was highly expressed when the bacterium first encountered the uranium, but that expression plateaued and then declined by the end of the growth-arrest phase. Together, these results strongly suggest *C. crescentus* is detoxifying the uranium throughout the course of the growth-arrest period.

To better understand how detoxification occurs, the biologists collected media from *C. crescentus* cultures grown in the presence and absence of uranium at various growth stages and added those samples to new cultures with fresh growth media and uranium. Growth media gathered during or after the growth-arrest period shortened the new culture's growth arrest and reduced expression



Caulobacter crescentus has a distinctive life cycle during which the bacterium undergoes asymmetric cell division into a mobile swarmer cell and a stationary stalked cell. These scanning electron microscope images show *C. crescentus* cells grown (a) without and (b) with uranium exposure. The cells exposed to uranium have a shorter stalk length, which suggests that uranium exposure delays the cell development and division processes.



Livermore researchers propose two scenarios to explain how metabolite secretion from *C. crescentus* protects cells from uranium toxicity. In the first scenario, the metabolite (blue squares) interacts with uranium (red circles) directly and either (1a) excludes uranium from the cell or (1b) sequesters it within the cell, thus preventing exposure to uranium toxicity. In the second scenario, (2) the metabolite mitigates the cell's uranium-induced stress response without physically interacting with uranium. (Rendering by Kwei-Yu Chu.)

of its uranium sensor gene—even for media taken from cultures that had never been exposed to uranium. The researchers concluded that *C. crescentus* produces a substance as part of some basic metabolic activity that helps to detoxify uranium. “The bacterium simply makes and secretes this metabolite throughout its life cycle,” says postdoctoral researcher Dan Park. “Our hypothesis is that the compound accumulates during the growth-arrest period, and at some point, the medium reaches levels of toxicity below that producing growth inhibition.”

A Change in Expression

In addition to observing the response of *C. crescentus* to uranium exposure at the colony level, the Livermore scientists delved more deeply into the bacterium itself, to pinpoint proteins and genes that may play a role in uranium resistance and detoxification. In 2005, Stanford University researchers performed a series of experiments on *C. crescentus* to determine how RNA expression changed in response to exposure to three heavy metals—uranium, cadmium, and chromium. Jiao's team, in conjunction with University of California at Davis researcher Brett Phinney, has since completed a complementary profiling study, looking at protein rather than RNA regulation.

Expression profiling measures the relative amounts of thousands of genes or proteins encoded by the genome at the same time. Protein expression levels of uranium-exposed cells collected during the growth phase were then compared with the levels of cells not exposed to uranium to distinguish uranium-specific expression.

While protein and RNA expression results matched in most respects, the protein study did reveal several insights. The team found that *C. crescentus* increased its expression of the protein

phytase fivefold when uranium was present. Phytase helps *C. crescentus* metabolize phytate, an abundant form of organic phosphorus found in the natural environment. In addition, two regulator proteins associated with the cell-division processes exhibited lower abundance when *C. crescentus* was exposed to uranium. These results are consistent with SEM imaging observations and the researchers' theory that cell development pauses as a result of uranium stress. “This study shows that the environment is affecting protein expression,” says Jiao. “Even

Microbiologist Yongqin Jiao is studying how some aerobic bacteria survive and even thrive in uranium-contaminated aquatic environments. (Photograph by George A. Kitrinos.)



though the bacterium eventually reproduces at the same rate as it does without uranium, the proteins are being disturbed.”

Jiao’s team has been collaborating with DOE’s Joint Genome Institute on a DNA study to ascertain which *C. crescentus* genes are important for uranium resistance. Using a comprehensive mutagenesis technique, the researchers engineered a large set of mutant *C. crescentus* cells. Each bacterium had a different single gene disrupted. Collectively, the approximately 4,000 genes of *C. crescentus*, except for a few hundred essential housekeeping genes, were individually rendered nonfunctional many times in the mutant pool. After exposing the mutants to uranium, they tallied the mutant survival rates using a comprehensive sequencing method. Those that did not survive likely had a gene disrupted that conveyed a survival advantage in the presence of uranium. The team is currently evaluating about two dozen gene candidates identified through the study, all of which, interestingly, are different than those found in the Stanford RNA study.

Precipitating a Discovery

Because phosphorus plays a key role in the survival of other uranium-resistant microorganisms, the team explored the phosphorus-related metabolic activity of *C. crescentus*. The researchers exposed *C. crescentus* cells to uranium and examined them with x-ray diffraction and transmission electron microscopy. Imaging showed that uranyl phosphate minerals had formed on the cell surface and in the surrounding medium. The researchers surmise that an enzyme located on a cell’s exterior, called extracellular phosphatase, aids in the formation of these minerals.

In growth media and the natural environment of *C. crescentus*, extracellular phosphatase converts various organic phosphates into

inorganic phosphates that the bacterium can absorb and use. In the presence of uranium, the researchers hypothesize that *C. crescentus* absorbs a portion of the inorganic phosphate released by the phosphatase for growth. The remaining phosphate likely binds with uranium on the cell exterior of *C. crescentus*, with the aid of phosphatase enzymes. The resulting uranyl phosphate mineral is less toxic and less soluble than the nonmineralized uranium.

Surprisingly, the researchers found that the extracellular phosphatase behavior occurs even without uranium exposure. Livermore postdoctoral researcher Mimi Yung observes, “The bacterium behaves this way naturally, and the presence of uranium neither promotes nor inhibits the activity.” Thus far, though, the researchers have been unable to link the increased phytase enzyme activity observed in the protein study to the mineral formation process.

To confirm that mineralization aided in the bacterium’s uranium tolerance and survival, the team deleted the gene responsible for extracellular phosphatase activity and uranyl phosphate formation. When the researchers exposed the modified and normal *C. crescentus* strains to uranium in the presence of organic phosphate, the modified bacterial cells died at a higher rate. While the phosphatase activity appears to be an innate property of the bacteria that is unaffected by uranium, the study confirmed that the cells do benefit from this activity when uranium is present.

Putting Bacteria to Work

Jiao’s team is building a convincing case for how *C. crescentus* metabolic activities can reduce the mobility and bioavailability of uranium. By the end of the study, Jiao, Yung, Park, and their collaborators hope to have gained an in-depth understanding of how *C. crescentus* interacts with uranium and changes the chemistry of its environment. The researchers expect many of the *C. crescentus* observations to be relevant to a broader spectrum of uranium-tolerant aerobic bacteria as well.

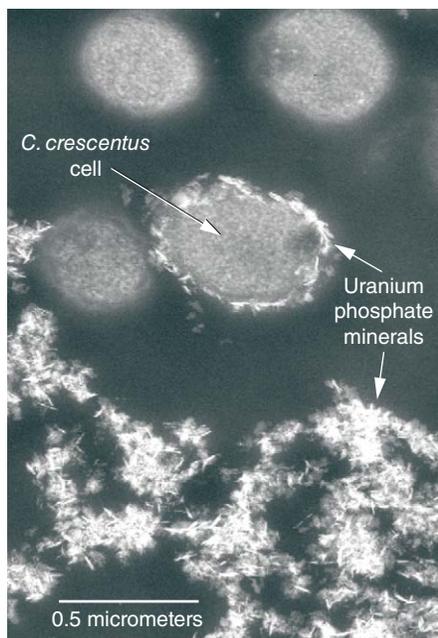
Research efforts by Lawrence Livermore and other institutions comprise the first, crucial step in improving uranium remediation. Once scientists understand how aerobic bacteria bioremediate uranium, they can begin to determine how to help the bacteria perform the job better, or even how to engineer better bacteria. These single-celled organisms could, in time, become formidable allies in toxic cleanup efforts.

—Rose Hansen

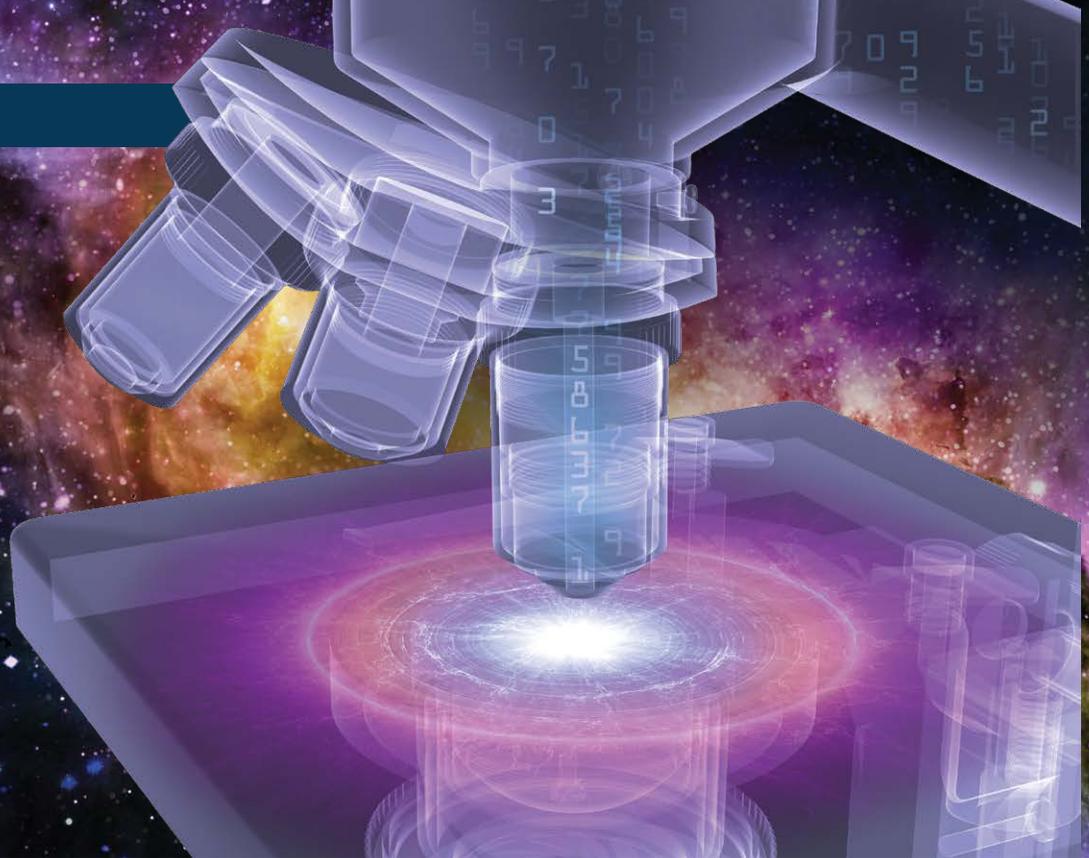
Key Words: bioremediation, *Caulobacter crescentus*, bacteria, Department of Energy (DOE) Early Career Research Program, expression profiling, gene disruption, metabolite, mutagenesis, phosphatase, phytase, toxic metal contamination, uranium, uranyl phosphate mineral.

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This transmission electron microscope image shows uranium phosphate minerals forming around and on the surface of *C. crescentus* cells, but not inside the cells (minerals appear brighter than the cells). *C. crescentus* produces an enzyme that aids in the formation of uranium phosphate minerals, which are less toxic and less mobile than the premineralized form of uranium.



Nuclear Fusion through a Computational Microscope



THE life of a star, from birth to death, is fueled by nucleosynthesis. At the heart of this process, nucleons—protons and neutrons—come together to form the atomic nuclei of virtually all the chemical elements in the universe. Nuclear fusion is a type of nucleosynthesis in which the nuclei of lightweight elements, such as hydrogen and helium, crash into each other and fuse, releasing large amounts of energy and creating the nuclei of heavier elements, for example, carbon and oxygen. These nuclear reactions are of great interest to astrophysicists who seek to answer the most fundamental questions about the origins of the universe and the evolution of stars.

Nuclear fusion reactions are very difficult to measure at the low energies relevant to stellar temperatures, primarily because the probability of two positively charged nuclei fusing together drops steeply with decreasing energy. Typically, scientists perform experiments at the lowest energy at which fusion reactions can be observed—from thousands down to hundreds of kiloelectronvolts—and then make theoretical extrapolations to lower energies of interest. However, the resulting estimated low-energy data may be unreliable because nucleon dynamics are disregarded in those calculations.

Livermore physicist Sofia Quaglioni is leading an effort to achieve a fundamental description of nuclear fusion using an *ab initio* (from the beginning) approach. “We are computing the properties of a system of nucleons viewed as pointlike particles that interact with each other,” says Quaglioni, who earned a 2011 Early Career Research Award from the Department of Energy (DOE) for her work. “We consider the force between nucleons and the laws of quantum mechanics to describe these microscopic systems.” The

scientific team, which includes Livermore postdoctoral researcher Guillaume Hupin and collaborators from TRIUMF in Canada and the Technische Universität Darmstadt in Germany, is developing a comprehensive framework using first-principles calculations and high-performance computing to describe dynamic processes between nuclei.

Many-body problems, such as the one studied by Quaglioni, are some of the most computationally intensive in science. To date, Quaglioni and her team have used more than 25 million core-hours on DOE supercomputers, with up to 100,000 cores per run. Those efforts have produced notable results, including pioneering work on nucleon–nucleus collisions and interactions of three nuclear fragments. The Laboratory’s 2014 Computing Grand Challenge Program has allocated the team an additional 2.5 million core-hours over the next year to further improve understanding of these complex physical phenomena.

Waves of Information

To study nuclear systems at a fundamental level requires an in-depth understanding of a system’s wave function, which is determined by solving the Schrödinger equation. The wave function describes the quantum state and behavior of the nucleons inside the nucleus. Protons and neutrons have a wavelike nature and thus have locations that can only be described by a probability distribution. The square modulus of the wave function—its absolute value squared—provides the probability density of finding the nucleons at a given position and time.

“When I joined the Laboratory as a postdoc in 2006, Livermore was at the forefront of developing methods to describe the wave

function of nucleons bound inside a nucleus,” says Quaglioni. “Since then, we have been working on the much more difficult problem of describing how nucleons behave in a system of two nuclei—a projectile and a target—with one colliding into the other.” In their model, the wave function is built as a linear combination of basis functions. A linear combination is the summation of a number of quantities, or terms. For a complex entity, such as a nucleus, the number of basis functions needed to describe all the possible states of component nucleons is very large. Correspondingly, the wave function describing the interaction of a projectile and a target, which requires multiplying the component linear combinations together, results in an expression with an enormous number of terms.

“Our model can often contain billions of terms,” says Quaglioni. “While more terms improve the accuracy of the model, they also make solving the Schrödinger equation more difficult.” Computational “superpower” is needed to antisymmetrize the basis functions so that two different nucleons do not occupy the same quantum states, which would violate the Pauli exclusion principle. Livermore’s high-performance supercomputers have opened the door for computationally intensive research such as Quaglioni’s. “Until just four years ago, an ab initio treatment of nuclear fusion was impossible,” she says. “With these powerful tools, we have begun to describe from first principles complex reactions such as the fusion of deuterium with tritium nuclei to produce helium-4 and a highly energetic neutron. We are now focused on taking this work to the next level.”

A Recipe for Theory

Fundamental interactions among nuclei are tied to the theory of quantum chromodynamics (QCD). QCD describes the “strong force” that holds quarks together to create composite particles known as hadrons, which include protons and neutrons. “Because quarks within nucleons are confined at energies relevant for nuclear physics, the nucleons themselves provide the correct degrees of freedom for the problem we want to solve,” says Quaglioni, who likens her approach to creating a recipe. “To

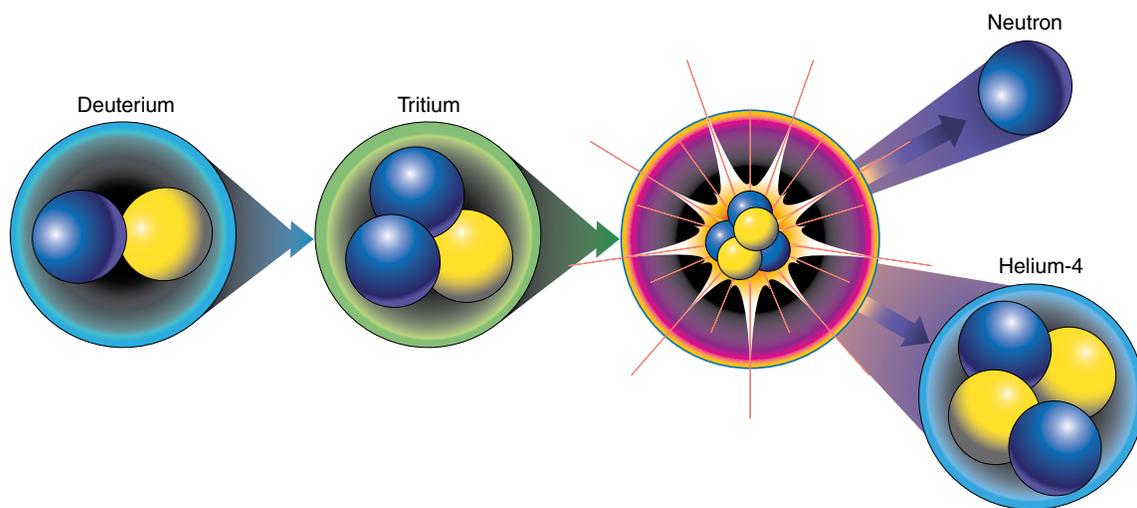
achieve the fundamental results we are looking for, we must have the right ingredients. Applying our knowledge of how the forces that bind nucleons together emerge from QCD is a key ingredient.”

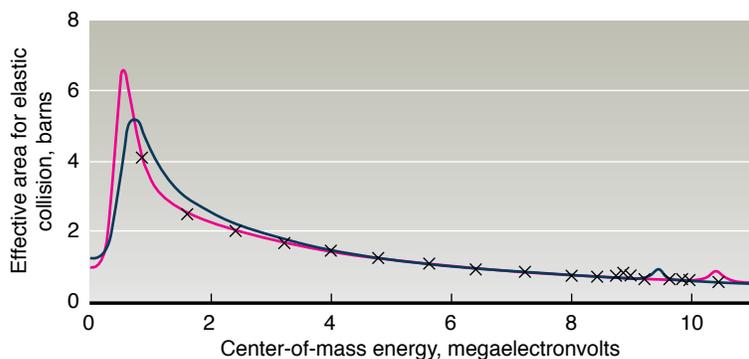
In this computational framework, the team incorporated nucleon–nucleon and three-nucleon forces, grounded in the underlying theory of QCD, via chiral effective field theory. The latter theory represents the interactions of hadrons in terms of field quantities varying in time and space. According to Quaglioni, part of what makes the nuclear many-body problem especially difficult is that the forces among nucleons have not yet been fully determined. These forces are much more complex than those of other microscopic systems such as atoms or molecules. Nucleons exert a strong attractive force between one another when they are a couple of femtometers (10^{-15} meters) apart, but they fiercely repel each other at even shorter distances. “Describing wave functions at these distances is challenging, because the calculations become harder to solve and require more basis states,” says Quaglioni. “Part of what makes this force especially complicated is that nucleons interact in triplets as well as in pairs.”

In the team’s first attempt at achieving an ab initio description of nuclear fusion, the researchers simplified the problem by omitting the three-nucleon force. The goal of Hupin’s postdoctoral research is to close the knowledge gap in this area by studying the effect of the three-nucleon force in low-energy nuclear reactions. Including the three-nucleon force—6 billion matrix elements that must be read and stored in memory—increases the computational burden dramatically. Another goal of Quaglioni’s team is to describe systems of three nuclei in relative motion. “Using the Laboratory’s supercomputers, we have radically improved our ability to describe collisions of two nuclei from first principles,” says Quaglioni. “With our most recent Grand Challenge allocation, we want to describe from first principles those systems that decay and emit three nuclei as well as reactions in which the target breaks apart, resulting in three nuclear fragments.”

To simulate dynamic interactions among nuclei, the team is combining the ab initio no-core shell model (NCSM) with the

An effort led by Livermore physicist Sofia Quaglioni used a first-principles approach to describe complex reactions such as the one depicted here. In this reaction, one of the protons in a deuterium (hydrogen-2) projectile is transferred to a tritium (hydrogen-3) target, leading to the formation of helium-4 and a highly energetic neutron.

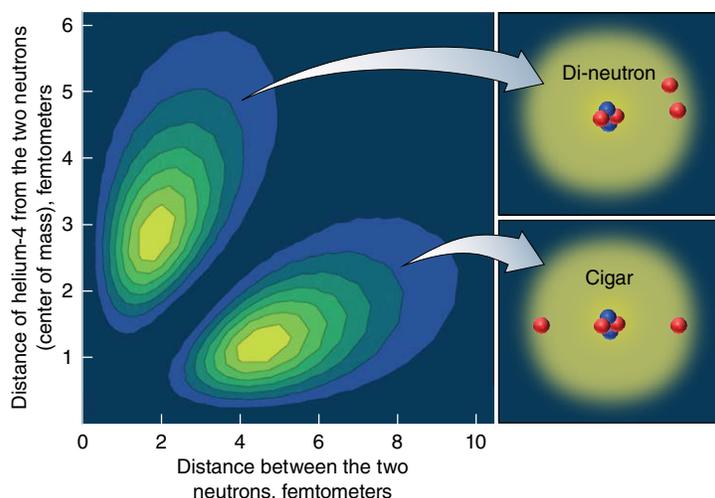




This graph shows the probability of a neutron's elastic scattering off a helium-4 target as a function of the kinetic energy of the particles' combined center of mass. Results obtained with the addition of the three-nucleon force (pink line) are significantly closer to experimental data (x) than results obtained with the nucleon-nucleon force (blue line) alone, confirming the importance of the three-nucleon force for describing these nuclear systems.

resonating group method (RGM). NCSM describes the internal structure of nuclei, called clusters, while RGM is a microscopic technique for describing the quantum mechanical interactions between the nuclei as well as clustering effects. With the extended NCSM-RGM, the team has accurately simulated the elastic scattering of neutrons, protons, and deuterium nuclei of helium-4 using nucleon-nucleon plus three-nucleon forces from chiral effective field theory. They have also described three-body cluster configurations of helium-6, in which a helium-4 nucleus interacts with two "halo" neutrons that orbit the nucleus at a distance.

"Two-nucleon halo nuclei have fascinated nuclear physicists for more than 25 years," says Quaglioni. "They are unstable nuclei. If we remove one of the three components—a nuclear core and two nucleons—the whole system falls apart. Because their constituents do not bind in pairs, we can better describe halo nuclei when their



The ab initio framework allows for all possible configurations of helium-6. The probability distribution function (left) shows the two most likely configurations: (top right) the Di-neutron configuration, which has two neutrons orbiting together far from the helium-4 nucleus, and (bottom right) the Cigar configuration, with two neutrons orbiting far apart from each other.

configuration is explicitly represented in the mathematics." This work represents the first-ever description of three-cluster dynamics within an ab initio framework. "The extension of NCSM-RGM to the treatment of three-body clusters will allow us to study not only halo nuclei but also reactions that end with three nuclear fragments," adds Quaglioni.

The team is leading an investigation into the unbound resonances of the helium-6 nucleus, which has already returned exciting results. "Our theory describes the first three positive-parity states of helium-6 in agreement with experiments, and it predicts the existence of new resonances that have not yet been measured," says Quaglioni. "We are thrilled that our ambitious idea for simulating complex, three-body systems works so well."

The Cosmos Revealed

Quaglioni and her team are one of the foremost groups combining first-principles approaches with high-performance computing to describe nuclear properties and improve nuclear theory. She says, "Today, accurate nucleon-nucleon and three-nucleon interactions from the chiral effective field theory offer a much desired link to QCD at low energies, helping us discover the true nature of the forces among nucleons and their role in star formation and evolution."

By enhancing the predictive capability of stellar modeling, this work is foundational to many Laboratory missions and supports fusion research at facilities such as the National Ignition Facility. A greater knowledge of the fundamental processes that fuel our stars enhances astrophysics research and may help reveal the secrets of elusive and enigmatic processes that have shaped and continue to form our universe.

—Caryn Meissner

Key Words: Computing Grand Challenge Program, Department of Energy (DOE) Early Career Research Award, fusion, no-core shell model (NCSM), nucleon, nucleosynthesis, quantum chromodynamics (QCD), resonating group method (RGM).

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Chemistry in Motion: Solving Big Problems with an Ultrafast Code

AS the world draws down the fossil fuel supply, “do more with less” has become a mantra in many fields, including energy and transportation. Meeting this challenge requires innovative approaches to solving some very big problems that occur on very small timescales. One important focus area is the design of efficient, environmentally friendly engines for transportation. Rather than relying on high-temperature combustion control methods, such as gasoline spark plugs and diesel injection, researchers designing next-generation engines are seeking to control the ignition process through alternate means that will enable much lower combustion temperatures.

In laboratory experiments, engines operating in low-temperature combustion modes have proven to provide high-efficiency power with low emissions of soot and nitrogen oxides. To better understand and develop these advanced concepts, engineers and designers must turn to computer codes that can resolve thousands of intermediate chemical species. Such codes exist but are, for the most part, very slow. They can require nearly a day to resolve a few seconds of reactions in a simplified simulation of gasoline combustion, thus limiting their usefulness in the engine-design process.

Livermore engineer Matthew McNenly has devised a solution to this conundrum: an innovative computational method that speeds up modeling the behavior of chemical systems by a factor of 1,000 over those methods traditionally used for internal combustion engine research. For those designing next-generation engines based on conventional transportation fuels and newer biofuels, his work will provide insight into the chemistry of fuel reactions, producing results in days instead of years.

Problems of Scale

When simulating complex systems in which many chemical reactions occur simultaneously, such as in combustion engines and nuclear reactors, the range of timescales proves to be a significant challenge. “We need to examine a host of reactions, from those faster than a femtosecond to those slower than a millisecond,” explains McNenly.

At the femtosecond (10^{-15} -second) scale, the key combustion reactions occur when a single molecule rearranges itself

According to the United Nations Environment Programme, failure to control soot emissions leads to an estimated 2 million premature deaths per year worldwide. In the U.S. and the European Union, 70 percent of soot emissions are from diesel engines. Developing efficient, environmentally friendly low-temperature combustion engines would reduce these and similar pollutants.

(isomerization) or falls apart into two or more products (decomposition). The speed at which these unimolecular reactions evolve is generally dependent on temperature, pressure, and mixture composition. “Resolving the competition between these ultrafast unimolecular pathways is crucial to designing low-temperature combustion engines,” says McNenly.

Reactions that are slower but just as critical occur between the nanosecond (10^{-9} -second) and microsecond (10^{-6} -second) scales. “In this time range, fluid dynamics is a relevant process,” explains

McNenly. Accurately simulating how chemical and fluid dynamic processes influence each other is a new area of research for McNenly and colleagues.

At the millisecond (10^{-3} -second) scale, the chemical pathways of interest are affected by the piston motion of the engine. Some important nitric oxide and soot formation pathways occur over milliseconds.

Another computational challenge is studying the interaction of the hundreds or thousands of chemical components contained in conventional hydrocarbon fuels (gasoline, diesel, or jet). The oxidation of each component may, in turn, involve thousands of intermediate species interacting through tens of thousands of reaction pathways. The traditional method for solving these large, complex systems involves commercial software codes that depend on “dense matrix solvers” for the heavy-duty computing. “These matrices are used to solve a problem in many dimensions, with the goal of determining what the new composition is at the completion of each time step,” says McNenly.

Even high-performance supercomputer systems, such as those at Livermore, take a long time to “step through” the solutions for large, detailed reaction networks using these traditional methods. For some of the reaction networks developed at Livermore, a calculation can take an entire day. Researchers have long sought methods to reduce the time to perform such calculations. Typically, the focus has been on reducing the network size by tracking fewer chemical species or by shrinking the number of reactions under consideration. However, accuracy is difficult to maintain with these approaches unless users have considerable expertise.

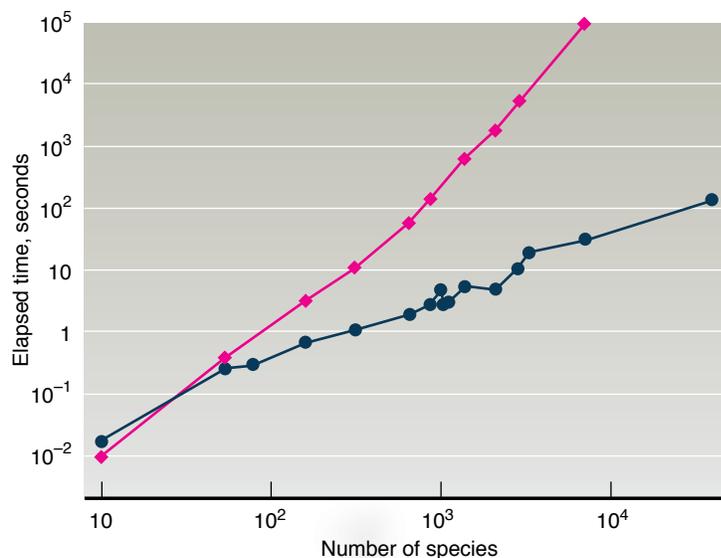
Engine of Change

About five years ago, while running a simulation of an engine model in support of the Laboratory’s combustion research effort, McNenly had an “aha” moment. As expected, the simulation was taking a very long time, even with the power of Livermore’s supercomputers. McNenly thought there must be a better way and began exploring concepts he had learned in a mathematics course as a graduate student. “The professor had taught us some interesting ways to solve certain kinds of linear problems,” he says. “Basically, rather than trying to solve the problem directly in its exact form, we took an iterative approach. The convergence to the exact solution is accelerated at each step by applying a preconditioner, which is a simplified form of the original problem and easier to solve.”

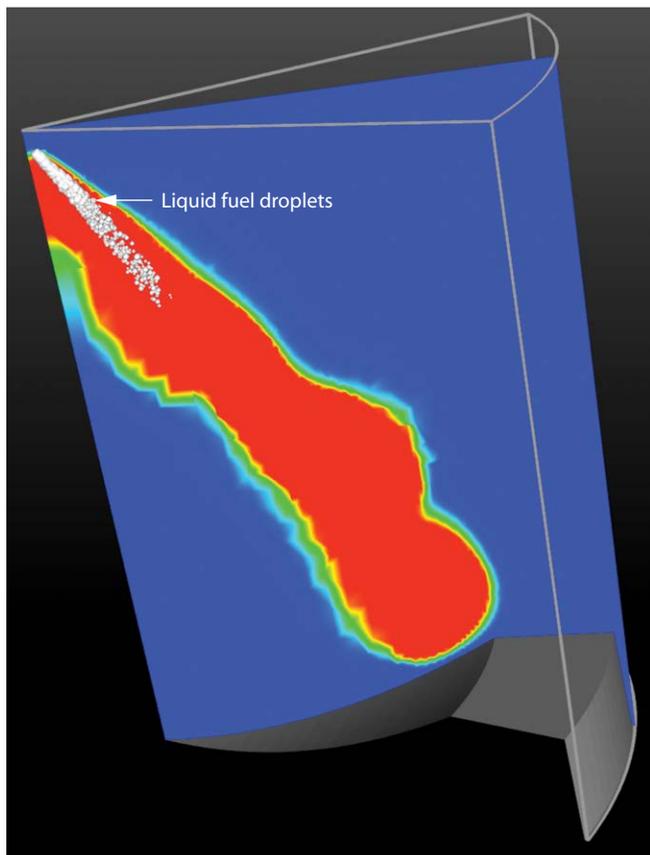
With support from the Department of Energy’s (DOE’s) Office of Energy Efficiency and Renewable Energy, Vehicle Technologies Program, McNenly pursued this intriguing concept for solving

large, complex chemical reaction networks. McNenly notes that his involvement in the DOE Computational Science Graduate Fellowship Program also helped make this work possible. “The fellowship program focuses on training graduate students in how to use DOE supercomputer systems for scientific research,” he says. “I was exposed to a broad range of numerical methods and algorithms, which made it possible for me to pursue this line of reasoning.”

McNenly’s method involves using matrix preconditioners to form highly efficient, sparse approximations to the reaction network. These preconditioners adapt “on the fly” to represent the most important reaction pathways at specific locations in the engine and at specific times during the combustion process. “Generally speaking,” says McNenly, “this approach identifies which reaction pathways are not important at a particular time and uses the preconditioner matrix to filter them out. For example, if the original fuel has reacted to form shorter intermediate species, the chemical pathways containing the original fuel composition are no longer needed and can be ignored. Our working hypothesis is that only a small number of reactions are needed to calculate from time A to time B. The critical reactions might change for time B to time C, but at that point, some reactions can be dropped and others added.”



Livermore researcher Matthew McNenly’s adaptive preconditioner (blue) outperforms traditional dense matrix solvers (pink) by three orders of magnitude, allowing the preconditioner to handle thousands of species at far less computational cost and without a loss of accuracy.



This engine design simulation shows the relative concentration (where red is the highest and blue the lowest) of iso-octane fuel after an initial injection event in a 45-degree slice of a Cummins B5.9 cylinder (each slice captures a single hole of an eight-hole fuel injector). The fuel is simulated using an 874-species mechanism, developed by Livermore's Bill Pitz and others, with a flow resolution of 200,000 fluid dynamic cells. With the new preconditioner, this very detailed mechanism can be used to simulate one engine design iteration in less than a day on 24 processors.

The important pathways are then mathematically represented in the sparse, preconditioner matrices. Because fewer pathways are represented, the simulation of reaction networks is accelerated tremendously. With McNenly's method, a simulation that took an entire day to run with traditional methods now takes less than 30 seconds. Even when compared to sophisticated commercial chemistry packages built on sparse solvers, McNenly's approach shows a fifteenfold improvement in time to complete a simulation. Most importantly, McNenly's method accomplishes these simulations without a loss of accuracy.

The Path Forward

McNenly's method is perfectly suited to speed up some fuel combustion simulations developed by researcher Bill Pitz, one of McNenly's colleagues at Livermore. Pitz and his collaborators have developed advanced hydrocarbon chemistry mechanisms that resolve the tens of thousands of critical reaction steps occurring during the combustion of transportation fuels. This level of detail is necessary to predict ignition and emission qualities in engine simulations. However, the mechanisms are too large to be used in a typical design simulation in industry, where supercomputing power and fast run times are not as readily available. "Our goal is to package these algorithms so those in private industry can easily use them to simulate advanced high-efficiency, low-emission engines during design cycles," says McNenly.

Thanks to the efforts of Livermore's Russell Whitesides and Dan Flowers (funded under a partner project), the solver has been implemented and licensed to one commercial software vendor. Other interested commercial entities include manufacturers of automobile and jet engines. Beyond these immediate applications, McNenly sees promise for any field in which interaction networks are paramount, including nuclear energy, biological systems, plasma dynamics, and astrophysics. He concludes, "We believe this approach can be helpful to anyone who is looking at what happens when two things collide, when the possibility of that collision is driven by concentrations."

—Ann Parker

Key Words: biofuel, chemical reaction network, diesel fuel, gasoline, internal combustion engine, low-temperature combustion, matrix solver, nitrogen oxide, preconditioner, soot.

For further information contact Matthew McNenly (925) 424-6418 (mcnenly1@llnl.gov).

In this section, we list recent patents issued to and awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Inductrack III Configuration—A Maglev System for High Loads

Richard F. Post

U.S. Patent 8,578,860 B2

November 12, 2013

Inductrack III configurations are suited for use in transporting heavy freight loads. Inductrack III addresses a problem associated with the cantilevered track of the Inductrack II configuration, which could present mechanical design problems in track systems that support heavy loads. In Inductrack III, the levitating Halbach array on the moving vehicle is single-sided and thus does not require the cantilevered track used with Inductrack II. As a result, the levitating portion of the Inductrack III track can be supported uniformly from below.

Melt-Castable Energetic Compounds Comprising Oxadiazoles and Methods of Production Thereof

Philip F. Pagoria, Mao X. Zhang

U.S. Patent 8,580,054 B2

November 12, 2013

In one embodiment, a melt-castable energetic material comprises at least one of two compounds: 3,5-bis(4-nitro-1,2,5-oxadiazol-3-yl)-1,2,4-oxadiazole (DNFO) or 3-(4-amino-1,2,5-oxadiazol-3-yl)-5-(4-nitro-1,2,5-oxadiazol-3-yl)-1,2,4-oxadiazole (ANFO). In another embodiment, a method for forming a melt-castable energetic material includes reacting 3,5-bis(4-amino-1,2,5-oxadiazol-3-yl)-1,2,4-oxadiazole (DAFO) with oxygen or an oxygen-containing compound to form a mixture of at least DNFO or ANFO.

Barium Iodide and Strontium Iodide Crystals and Scintillators Implementing the Same

Stephen A. Payne, Nerine J. Cherepy, Giulia E. Hull,

Alexander D. Drobshoff, Arnold Burger

U.S. Patent 8,580,149 B2

November 12, 2013

In one embodiment, a material comprising a crystal of strontium iodide (SrI_2) provides at least 50,000 photons per megaelectronvolt (MeV). In another embodiment, a scintillator radiation detector includes a scintillator optic made of europium- (Eu-) doped strontium iodide, which provides at least 50,000 photons per MeV. Another radiation detector design includes a scintillator optic of SrI_2 and barium iodide (BaI_2), wherein the ratio of SrI_2 to BaI_2 is in the range of 0:1. The method for manufacturing a suitable crystal for the scintillator involves mixing SrI_2 -containing crystals with a source of Eu^{2+} , heating the mixture above a melting point of the SrI_2 -containing crystals, and cooling the heated mixture near the seed crystal for growing a crystal. Additional materials, systems, and methods are presented.

Corrosion Resistant Neutron Absorbing Coatings

Jor-Shan Choi, Joseph C. Farmer, Chuck K. Lee, Jeffrey Walker,

Paige Russell, Jon Kirkwood, Nancy Yang, Victor Champagne

U.S. Patent 8,580,350 B2

November 12, 2013

With this method, a corrosion-resistant, neutron-absorbing coating is applied to a material by a spray, deposition, sputtering, or welding process to form a composite material. A corrosion-resistant, neutron-absorbing coating comprising a composite material can also be made of a spray, deposition, sputtering, or welding material and a neutron-absorbing material.

Monolithic Three-Dimensional Electrochemical Energy Storage System on Aerogel or Nanotube Scaffold

Joseph C. Farmer, Michael Stadermann

U.S. Patent 8,580,438 B2

November 12, 2013

A monolithic three-dimensional electrochemical energy storage system is provided on an aerogel or nanotube scaffold. An anode, separator, cathode, and cathodic current collector are deposited on the aerogel or nanotube scaffold.

Magnetic Bearing Element with Adjustable Stiffness

Richard F. Post

U.S. Patent 8,581,463 B2

November 12, 2013

A compact magnetic bearing element is made of permanent magnet discs configured such that bearing stiffness and levitation force can be varied over a wide range.

Methods of Detection and Identification of Carbon- and Nitrogen-Containing Materials

Alexander Ivanovich Karev, Valery Georgievich Raevsky,

Leonid Zavenovich Dzhilavyan, Louis Joseph Brothers,

Larry K. Wilhide

U.S. Patent 8,582,712 B2

November 12, 2013

Methods for detecting and identifying carbon- and/or nitrogen-containing materials are disclosed. The methods may detect photonuclear reaction products of nitrogen and carbon to identify the carbon- and/or nitrogen-containing materials.

Separating and Combining Single-Mode and Multimode Optical Beams

Anthony J. Ruggiero, Donald A. Masquelier, Jeffery B. Cooke,

Jeffery S. Kallman

U.S. Patent 8,582,936 B2

November 12, 2013

These techniques can be used to combine initially separate single-mode and multimode optical beams into a single dual-mode fiber optic. Bidirectional propagation of two beams that are differentiated only by their mode profiles (that is, by wavefront conditions) is provided. The beams can be different wavelengths and have different modulation information but still share a common aperture. This method allows the use of conventional micro-optics and hybrid photonic packaging techniques to produce small rugged packages suitable for industrial or military environments.

Physics-Based Signal Processing Algorithms for Micromachined Cantilever Arrays

James V. Candy, David S. Clague, Christopher L. Lee, Robert E. Rudd, Alan K. Burnham, Joseph W. Tringe

U.S. Patent 8,584,506 B2

November 19, 2013

This method uses physics-based signal-processing algorithms for micromachined cantilever arrays. With this approach, the deflection of a micromachined cantilever represents the chemical, biological, or physical element being detected. One embodiment includes steps for modeling the cantilever deflection, sensing the deflection of the micromachined cantilever, and producing a signal that represents this deflection. The deflection signal is then compared with the deflection model to identify the element.

Low Temperature Sodium-Beta Battery

Joseph C. Farmer

U.S. Patent 8,586,227 B2

November 19, 2013

A battery designed to operate at ambient temperature or lower has a current collector, a sodium eutectic anode, and a low-melting ion liquid cathode within an enclosure and a separator and electrolyte between the anode and cathode. The anode and cathode are made of materials that are in a liquid state at ambient temperature or lower and thus will operate at these low temperatures.

Awards

Laboratory physicist **Miguel Morales** received a 2014 **Presidential Early Career Award for Scientists and Engineers (PECASE)** for his leading-edge research in condensed-matter physics. This honor is the highest bestowed by the **U.S. government** on outstanding scientists and engineers, who are early in their independent research careers. Using advanced computational techniques such as density functional theory and quantum Monte Carlo, Morales studies materials at extreme pressure and temperature on some of the world's most powerful supercomputers. His work is important to stockpile stewardship, the National Nuclear Security Administration's program to ensure the safety and reliability of the nation's nuclear weapons stockpile. In addition, his research provides planetary scientists with a better understanding of planet formation. PECASE winners receive \$50,000 a year over five years to pursue research in their field.

Lawrence Livermore scientist **Steve Payne** was selected as a **fellow** by the international optics and photonics society **SPIE**. Founded in 1955, SPIE serves engineers and scientists in government, academia, and industry in the fields of optics, photonics, and light. The nonprofit selected Payne for his research contributions and new discoveries in these fields. Payne is the associate program leader for radiation detection materials in the Global Security Principal Directorate. His research interests

include radiation detectors, materials, optics, and lasers. Several of the materials that he and his colleagues have developed are commercially available, including the high-resolution $\text{SrI}_2(\text{Eu})$ gamma detector and the first plastic capable of efficiently distinguishing neutrons from gamma rays. (See *S&TR*, October/November 2012, pp. 10–11.) Payne uses experimental and theoretical methods to explain the physics of scintillators and is recognized as a key architect of the roadmap for understanding the mechanisms.

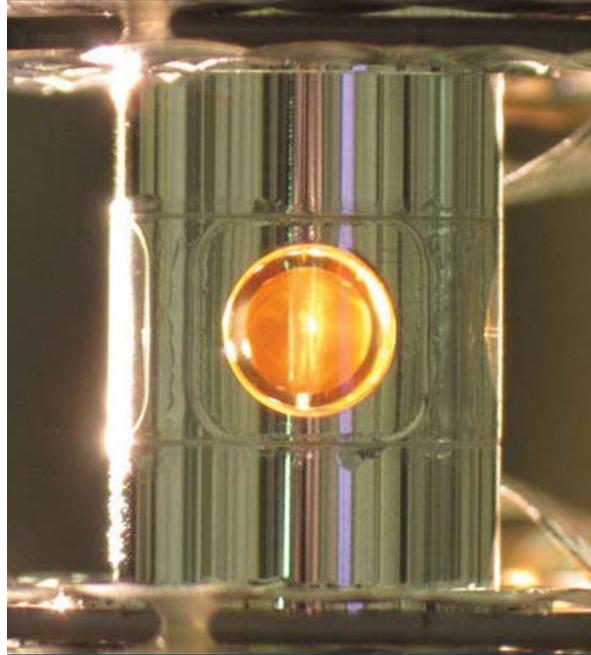
Dona Crawford, associate director of Livermore's Computation Directorate, was selected as a **member** of the **California Council on Science and Technology (CCST)**. The council is an assembly of corporate executives, academics, scientists, and scholars who are leaders in their respective fields. CCST members provide expert counsel on science and technology issues facing California. Says Crawford, "As an applied science laboratory, we can both contribute and benefit from the work of the CCST. By participating, we can build on our long-standing relationship with the state as a part of the University of California. Many of the challenges the state faces, such as energy, environment, and cybersecurity, also are national concerns that are the focus of Livermore missions." Crawford has been appointed for a three-year term, renewable for a second term.

Predicting Wind Power with Greater Accuracy

Wind power in the U.S. is growing at a rapid clip and is competitive with other alternate forms of power generation. However, the wind is a variable and uncertain power source that is dependent on many complex atmospheric forces. Reducing the uncertainty of wind power forecasts used by the wind farm industry and electric grid operators, is the goal of a team of Lawrence Livermore atmospheric scientists, mechanical and computational engineers, and statisticians. The team's advanced computer models, verified by fieldwork and statistical analysis, account for atmospheric complexities both horizontally across landmass and vertically above Earth's surface. These high-resolution computer simulations are providing more useful information to wind farm developers and operators, electric power grid operators, and wind turbine manufacturers.

Contact: Wayne Miller (925) 424-4472 (miller99@llnl.gov).

A Big Step toward Ignition



Recent experiments at the National Ignition Facility are achieving record neutron yields and much better consistency with models.

Also in June

- *An innovative time projection chamber measures neutron-induced fission cross sections in actinides with unprecedented accuracy.*
- *A sensor based on tangled arrays of double-coated carbon nanotubes provides a reliable method for detecting trace amounts of chemicals in the environment.*
- *Livermore climate researchers find that human activities may be changing precipitation on a global scale.*

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